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E.W. Heinonen & R.E. Tapscott

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The University of Mexico
Albuquerque, NM 87131-1376

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Wright Laboratories
132 Barnes Drive, Suite 2
Infrascructure Technology Section
Tyndall Air Force Base, FL 32403-5319

SERDP
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Arlington, VA 22203

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USAF/AAWG/CGET ADVANCED AGENT REFERENCE Database Description

Everett W. Heinonen and Robert E. Tapscott

Center for Global Environmental Technologies
NEW MEXICO ENGINEERING RESEARCH INSTITUTE
The University of New Mexico
Albuquerque, New Mexico 87131-1376

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WRIGHT LABORATORIES (WL/FIVCF)
139 Barnes Drive, Suite 2
Infrastructure Technology Section
Tyndall Air Force Base, Florida 32403-5319

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ROBERT A. TETLA
Project Officer

EDGAR F. ALEXANDER
Chief, Air Base Technology Branch

RICHARD N. VICKERS
Chief, Infrastructure Technology Section

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The University of New Mexico
Albuquerque, New Mexico 87131-1376

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In 1993, production of halon fire and explosion protection agents was phased out and to date, no Halon 1301 substitute has been identified to provide total-flood protection against fires and explosions in normally occupied areas without major changes in system hardware. A study was begun to assess the probability of success and to determine the most promising directions for development of new chemical alternatives to Halon 1301. A database entitled the USAF/AAWG/CGET ADVANCED AGENT REFERENCE Database was established as a repository of summary information on documents relating to advanced agents. This report describes the structure and organization of the database, and provides images of the major forms used to present the data, which includes a complete bibliographic citation, abstract, and text blocks for conclusions on potential agent use and evaluation of the concept presented in the paper. The data are stored in a companion database, the NMERI LIBRARY Database.

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PREFACE

This report was prepared by the Center for Global Environmental Technologies (CGET), New Mexico Engineering Research Institute (NMERI), The University of New Mexico, Albuquerque, New Mexico, for the Advanced Agent Working Group (AAWG) under Contracts 91AU225P, NMERI Number 30930; F08635-93-C-0073, NMERI Numbers 31882 and 31883; and BI305006UQ, NMERI Number 32350. This document provides the Final Report for Advanced Agent Identification and Preliminary Assessment.

The project Start Date was 9 January 1995, and the End Date was 16 November 1995. The AAWG member organizations are the North Slope Halon Task Group; the U.S. Army - TACOM, the U.S. EPA, Stratospheric Protection Division; Wright Laboratories (WL/FIVCF); and 3M Company. Contacts and representatives from the member organizations are David Catchpole, BP (Exploration) Alaska representing the North Slope Halon Task Group; Charles J. Kibert and Capt Robert A. Tetla, Wright Laboratories (WL/FIVCF); Steve McCormick, U.S. Army TACOM; Karen Metchis, US EPA; and Scott D. Thomas, 3M. The NMERI Principal Investigator is Robert E. Tapscott.

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EXECUTIVE SUMMARY

A. OBJECTIVE

The objective of this study is to assess the probability of success and to determine the most promising directions for development of new chemical alternatives to Halon 1301 in fire suppression and explosion prevention and suppression applications. The portion of this work discussed herein describes a database to contain references to advanced agent firefighting agents.

B. BACKGROUND

On 31 December 1993, production of halon fire and explosion protection agents was phased out in all developed nations under requirements imposed by the Montreal Protocol, an international treaty. To date, no Halon 1301 substitute has been identified to provide total-flood protection against fires and explosions in normally occupied areas without major changes in system hardware. To lay a foundation for development of such agents requires answers to four questions: (1) What mechanisms are available for chemically active agents (CAAs) for protection against fires and explosions? (2) Based on these mechanisms, what families of chemicals could provide an advanced replacement for Halon 1301? (3) What is the preliminary assessment of manufacturability, global environmental impact, and toxicity for these families? (4) Taking all of the above into account, what are the prospects for a halon replacement for a total flood explosion and fire protection of normally inhabited areas that would allow use without major hardware changes? To answer these four questions, the Advanced Agent Working Group (AAWG) — composed of participants from the U.S. Military, from users, and from industry — was established, and a research program instituted to provide the data. A database entitled The USAF/AAWG/CGET ADVANCED AGENT REFERENCE Database was developed to provide access to references on advanced agents.

C. SCOPE

To ensure that a thorough review of advanced agent technology is made, a comprehensive bibliography of all advanced agent references must be available. References found in many different journals, books, conference proceedings patent applications, and other sources were

found through extensive library searches, and a convenient method of storage and retrieval was developed.

D. METHODOLOGY

NMERI conducted a library search for references to advanced agents. A computerized database, the USAF/AAWG/CGET ADVANCED AGENT REFERENCE Database, hereafter called the ADVANCED AGENT Database, was developed to store the references. This database includes a table of the references and a form that displays a complete bibliographic citation, keywords, and an abstract for each reference, as well as a page each for conclusions on the content of the reference and proposed concepts for firefighting. The ADVANCED AGENT Database is linked to the CGET/APT LIBRARY Database, which contains nearly 4000 references on ozone-depleting substance (ODS) replacement, firefighting chemicals and techniques, and related subjects. Only those references in the LIBRARY Database concerning aerosols are included in the ADVANCED AGENT Database, which can be distributed to users regardless of whether they have Microsoft Access on their computers. The ADVANCED AGENT Database can be searched for keywords or words in the text.

E. APPROACH

A total of 57 references have been included in the present version of the ADVANCED AGENT Database, which is designed to facilitate the addition of new references and searches of current references by topic.

F. RECOMMENDATIONS

It is recommended that the ADVANCED AGENT Database be updated as new advanced agent references are found to permit researchers in the field to have timely access to references on advanced agent technology.

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ABBREVIATIONS AND ACRONYMS

AAWG	Advanced Agent Working Group
ADT	Access Developer's Toolkit
CGET	Center for Global Environmental Technologies
NMERI	New Mexico Engineering Research Institute
ODS	Ozone-Depleting Substance
RDB	Relational Database
SQL	Structured Query Language
USAF	United States Air Force

SECTION I
INTRODUCTION

The USAF/AAWG/CGET ADVANCED AGENT REFERENCE Database (herein called the ADVANCED AGENT Database) provides complete bibliographic data, abstracts, conclusions, and potential applications on references relating to advanced agents that could replace halocarbons in firefighting, in the future. These compounds consist only of those designated as Second- and Third-Generation agents and do not include most of those being commercialized today, i.e., commonly referred to as First-Generation agents. The former compounds include the "Second-Generation" tropodegradable halocarbons and the "Third-Generation" non-halocarbon agents.

The ADVANCED AGENT Database has been designed to provide a single-source compilation for literature references concerning these compounds. Sources are journals, periodicals, reports, conference procedings, patents, and others. The database allows searches for references by any term in the bibliographic reference, by key words, or by terms in the abstract. The source documents from which the data are extracted are contained in the New Mexico Engineering Research Institute (NMERI) LIBRARY Database© (herein called the LIBRARY Database). The database is being continuously updated and will be made available to researchers.

The ADVANCED AGENT Database is a relational database (RDB) written in Microsoft Access (Reference 1) using a Windows environment. The entire database with an executeable program is being made available for distribution using the Access Developer's Toolkit (ADT) for Windows.

SECTION II

COMPUTERIZED DATABASE

Many references on the chemical and physical properties and performance of compounds that could replace ozone-depleting substances (ODS) are contained in periodicals, reference books, and manufacturers' information. However, up to this time, no single source contains a comprehensive listing of those references. To provide an accurate, convenient access to these references, a computerized RDB was designed to manage the storage, addition, and update of bibliographic and abstract data to allow retrieval of the source documents.

RDBs are sophisticated filing and cross referencing systems. Among the several advantages of RDBs are those listed below (Reference 2).

1. RDBs allow relations to be established between tables of data to eliminate problems with multiple changes and duplication. It is important that data changes not be required in more than one location. For example, each individual piece of information appears in only one place. Thus, a single change for a value applies to all locations of that data in forms, queries, etc.

2. RDBs allows informational exchange with other applications. For example, with appropriate software, the ADVANCED AGENT Database can "launch" data to word processing applications for compiling reports or inclusion in other documentation. In general, controls on the database are labeled "launch" for creation of a Word for Windows merge file, and "print" for printing reports directly from Access.

3. Structured Query Language (SQL) allows searches and compilations of data to be made rapidly and easily.

A. DATABASE STRUCTURE

The ADVANCED AGENT Database contains two types of entities: primary objects (Tables, Queries, Forms, Macros, and Modules) and control objects (where data are entered and displayed), which are often part of the former. Here, only primary objects are discussed.

1. Tables, which contain the data in fields, are the most important part of any database. Tables contain records which are made up of fields, such as the reference number or the conclusions.

2. Forms provide a convenient way to view, add, and change data in the tables. Forms are used primarily on the computer screen, although they can be printed out. Each separate datum on a form is contained in a control, which allows data entry or display.

3. Reports can be used to generate printed information from data in tables or data selected by queries.

4. Macros permit programming for conducting repetitive functions.

5. Modules employ computer language to carry out complex functions.

The various objects in an RDB (including control objects) are often named using a special convention (Reference 3), and that convention has been followed here for the primary objects and most, but not all, control objects. Each object is given a name that contains a tag and a Base. In addition, there may also be a prefix (rarely used) and a Qualifier. The names have the following form: [prefix]tagBase[Qualifier]. The prefix (if any) and the tag are lower case. The first letter of the Base and Qualifier are capitalized. Suggested tags are given in Table 1. Qualifiers are much less well defined; however, a few suggested qualifiers are shown in Table 2. Qualifiers are not used in the present version of the ADVANCED AGENT Database.

TABLE 1. TAGS FOR OBJECT NAMES.

Primary (Container) Objects		Control Objects	
Object	Tag	Object	Tag
Form	frm	Chart	cht
Macro	mcr	Check Box	chk
Module	mod	Combo Box	cbo
Query (Select)	qry	Command Button	cmd
Query (Append)	qrya	Frame	fra
Query (Crosstab)	qryc	Label	lbel
Query (Delete)	qryd	Line	lin
Query (Make Table)	qrym	List Box	lst
Query (Update)	qryu	Option Button	opt
Report	rpt	Option Group	grp
Table	tbl	Page Break	brk
		Shape	shp
		Subform	sfrm
		Text Box	txt
		Toggle Button	tgl

TABLE 2. COMMON QUALIFIERS.

Property	Qualifier
First Element of a Set	First
Last Element of a Set	Last
Next Element of a Set	Next
Previous Element of a Set	Prev
Lower Limit of Range	Min
Upper Limit of Range	Max
Source	Src
Destination	Dest

B. TABLES

A list of all tables in the ADVANCED AGENT Database is shown in Table 3. The ADVANCED AGENT Database has one primary table, **tblAdvanced**, which contains bibliographic and other data on each reference. The number of records in this table will change as additional records are added or deleted. The RDB permits relationships to be set up between tables of data to limit duplication of data and to decrease the chance for errors from the use of multiple entries. The table **tblTotalQ** contains data on publications and authors attached from the LIBRARY Database. The table **tblTotalQQ,** containing only those references actually used in the database, is generated for the distribution copy (in this and other databases designed by NMERI/CGET, the convention of adding a "Q" as a suffix is used when naming generated tables). The table **ztblLaunchQ** is generated by queries and is used only to contain final input for "launch" into word processing programs or into reports printed by Access. Note that this table is generated by more than one query and, therefore, the structure may change depending on the query used. This table does not contain permanent data.

TABLE 3. TABLES IN ADVANCED AGENT DATABASE.

Name	Number of Records*	Description
tblAdvanced	59	Reference numbers, conclusions, concepts, subjects
tblTotalQ	3997	Table of all references generated from the LIBRARY Database
tblTotalQQ	59	Table of only those references from **tblTotalQ** used in this database
tblLaunchQ	varies	Temporary table used in launching information to reports and word processing

* This is the number of records at the time this report was written; the totals will change as the database is expanded.

C. QUERIES

The ADVANCED AGENT Database contains the Make Table query **qrymLaunch**, (Table 4), which is used to generate a temporary table storing data from the single record to be launched to Word.

TABLE 4. QUERIES IN ADVANCED AGENT DATABASE.

Name	Type	Description
qrymLaunch	MakeTable	Used for launching individual records into Word for Windows

D. FORMS

Forms provide the major interface between users and the ADVANCED AGENT Database (Table 5).

When the database is opened, the **frmSwitchboard** form appears, allowing access to **frmAdvanced** and permitting launching or printing data. The form **frmAdvanced** is the principal form for the advanced agent reference table. This form allows the viewing, addition, deletion, and editing of data within those tables, as well as providing the capability to find

records. The form **frmAddRecordMod** allows selection of a record in the LIBRARY Database to be included in the ADVANCED AGENT Database by being appended to **tblAdvanced**. The form **frmFindMod** allows for the database to be searched for selection of records containing certain terms.

TABLE 5. FORMS IN ADVANCED AGENT DATABASE.

Name	Description
frmAddRecordMod	Allows addition of record to form via LIBRARY Database Reference Number
frmAdvanced	Prinicipal data entry and search form for database
frmBackground	Covers screen during time-consuming operations
frmFindMod	Find record popup
frmGlobal	Hidden form for temporary storage of variables
frmMenu	Temporary form used in Wordlaunch in the distributed copy
frmSwitchboard	Initial form displayed upon entry

E. REPORTS

The present ADVANCED AGENT Database will produce a number of printed reports (Table 6). The reports **rptAdvanced** and **rptList,** respectively, allow printing of reports containing a single page printout of each record and a compilation of bibliographic data for all records.

TABLE 6. REPORTS IN ADVANCED AGENT DATABASE.

Name	Description
rptAdvanced	One-page report of all data
rptList	Lists bibliographic references only

F. MACROS

The macros used by the ADVANCED AGENT Database are listed in Table 7. Note that, with the exception of **Autoexec**, each of these is actually a set of several macros with related functions.

The **Autoexec** macro sets up the database and brings up **frmSwitchboard** when the ADVANCED AGENT Database is first started. This macro also hides the database window, changes the window caption, and makes adjustments in the window. The macro **mcrChangeWindow** contains the macros that allow movement from one form to another; **mcrFind** contains all of the macros associated with finding specific records when the "Find Record" buttons are activated on a form; and **mcrForm** is a generalized set of macros used in manipulating forms. The macro **mcrLaunch** contains macros to print data in reports or to launch data to a Word for Windows merge file. The macro **mcrExportMenu** is only used in launching data in the distributed copy of the database.

TABLE 7. MACROS IN ADVANCED AGENT DATABASE.

Name	Description
Autoexec	Initializes system
mcrChangeWindow	Changes forms
mcrExportMenu	Used in launching data in distributed version of database
mcrFind	Group of macros for finding specific records
mcrForm	Manipulates forms including opening, closing, pagination
mcrLaunch	Launches data to reports and word processing

G. MODULES

The database uses four modules containing programs written in Access Basic (Table 8). The module **modCaptionOnly** and **modChangeCaption** establish the appearance of the screen with the name of the database at the top. The module **modMoveRecord** permits the use of certain buttons on forms to move between records. Finally, **modUtilities** is a general set of utilities used in the databases.

TABLE 8. MODULES IN ADVANCED AGENT DATABASE.

Name	Description
modCaptionOnly	Sets up window to eliminate menus, tool bars, scroll bars
modChangeCaption	Places caption on window
modMoveRecord	Generalized routines for paging through records
modUtilities	Assorted utilities

SECTION III
FORMS

Data entry, viewing, navigating, and output functions are conducted in forms. The major forms used in this database are discussed in detail below.

A. SWITCHBOARD FORM

The Switchboard form (**frmSwitchboard**) is displayed upon entry to the database (Figure 1). It contains five buttons that permit various operations (Table 9).

TABLE 9. BUTTONS IN FRMSWITCHBOARD.

Button	Function
"Advanced Agent References"	Opens the form **frmAdvanced**, which is the main data entry and viewing form for the database.
"Print Document List"	Prints a list of bibliographic records using **rptList.**
"Print all Document Information"	Prints a list of all records using **rptAdvanced.**
"Launch all Document References"	Opens the Access to Word utility, which allows the launching of records to a Word for Windows merge file
"Exit Microsoft Access"	Exits the database back to the window from which it was entered

B. ADVANCED FORM

The Advanced Agent form (**frmAdvanced**) is a long form that cannot be completely displayed on the screen (Figure 2. Form frmAdvanced Page 1). Therefore, it has been divided into the four "pages" independently displayed on the screen by selecting one of the four buttons on the form or "Page Up" or "Page Down" keys on the keyboard. The buttons in this form are illustrated in Table 10.

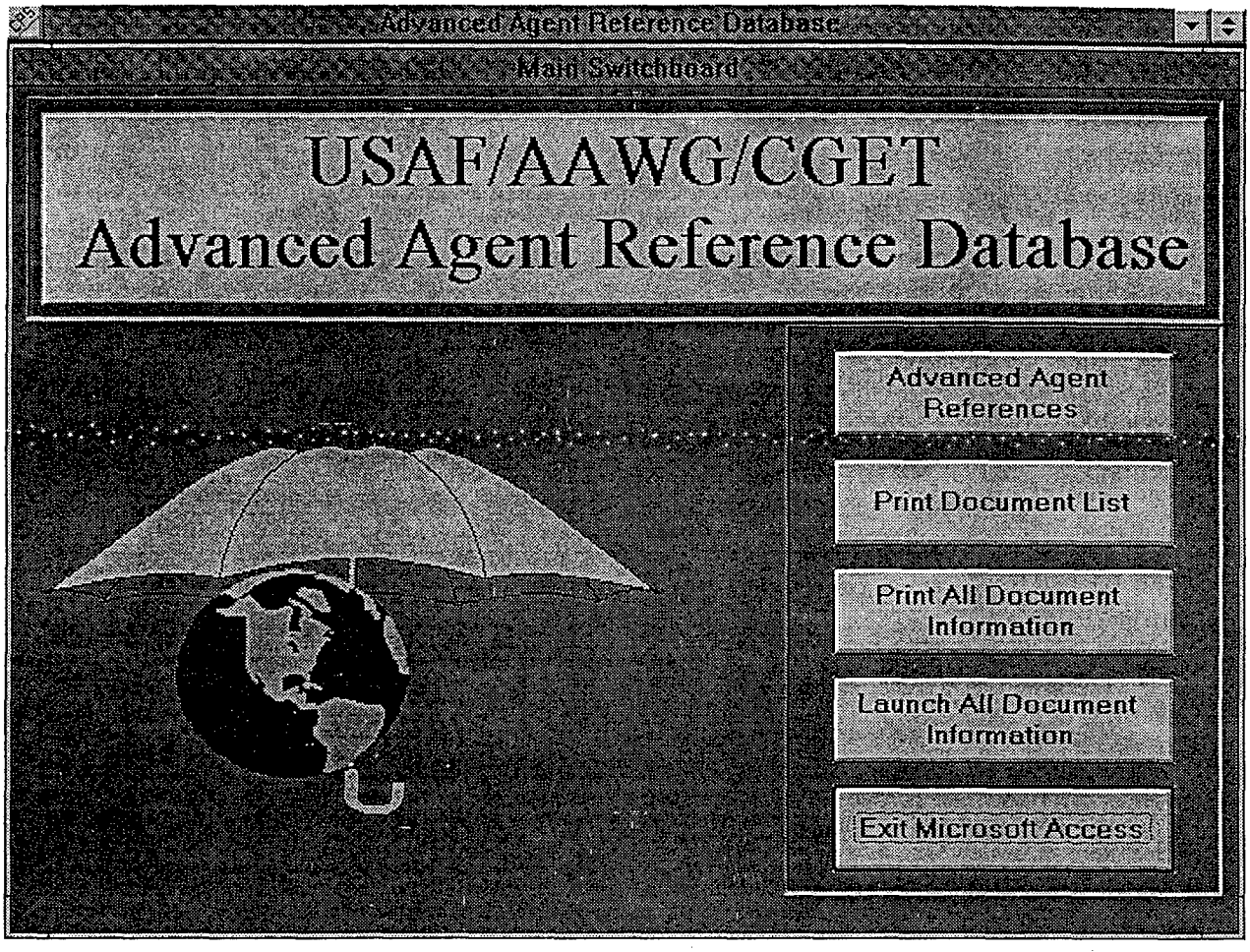

Figure 1. Form frmSwitchboard.

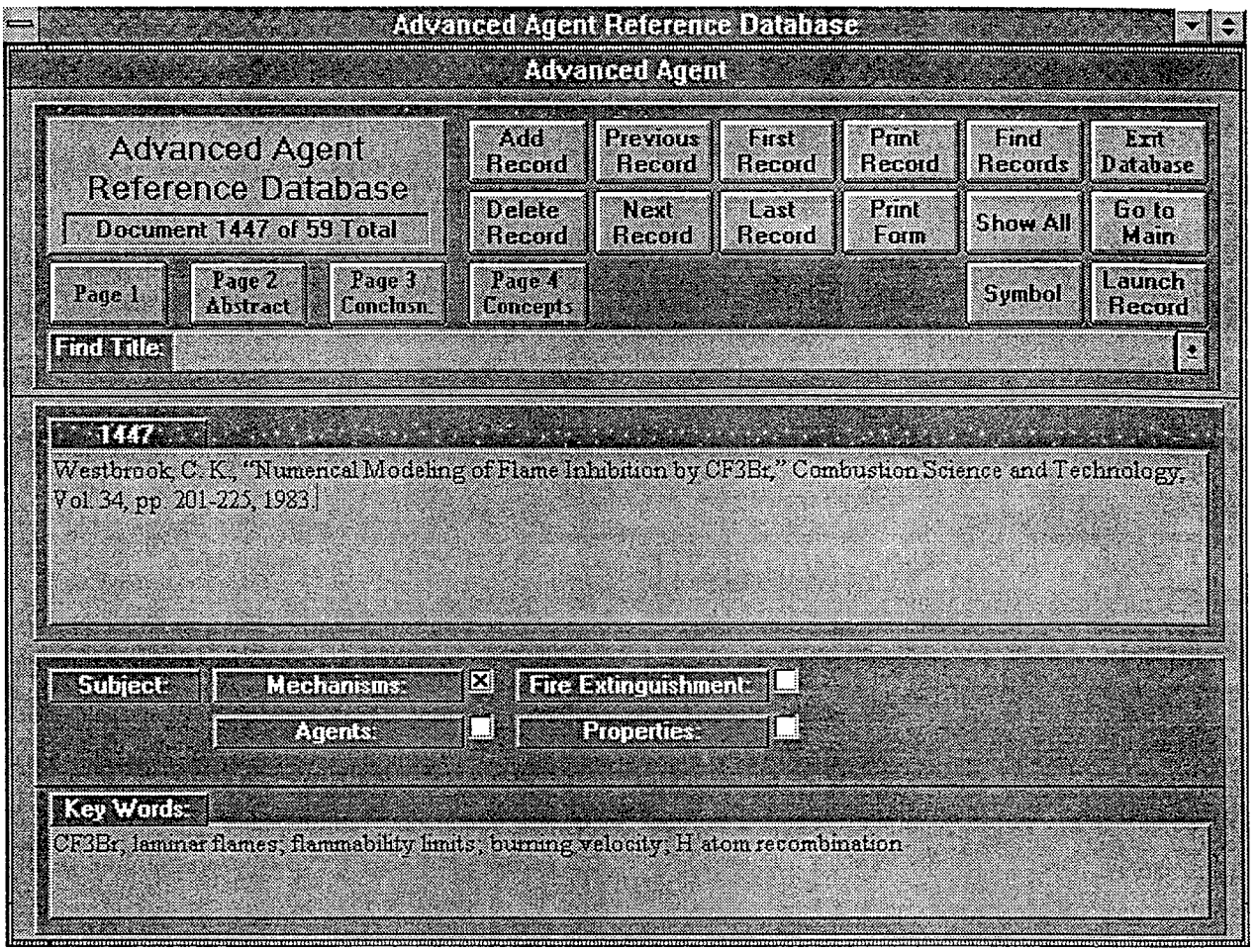

Figure 2. Form frmAdvanced Page 1.

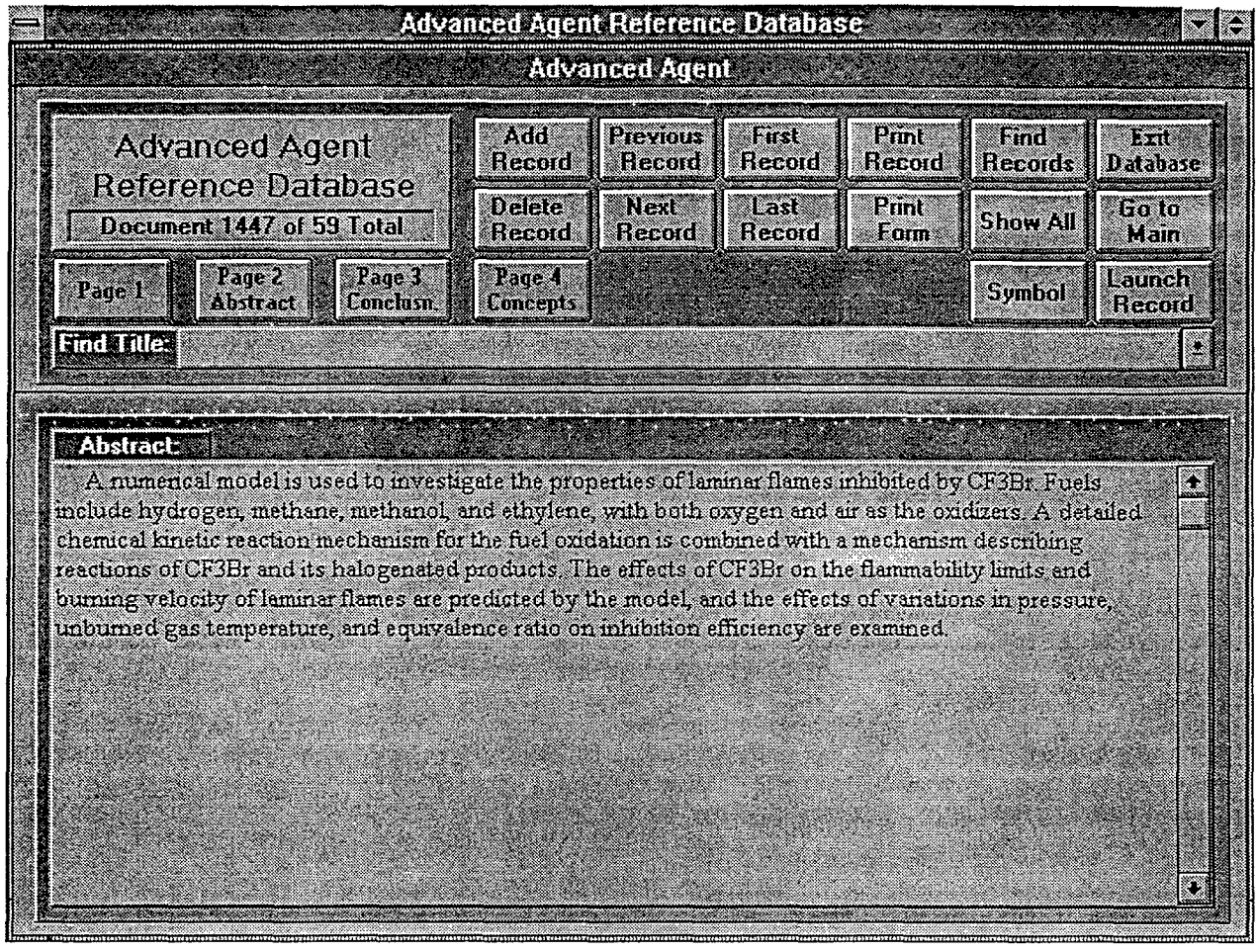

Figure 3. Form frmAdvanced Page 2.

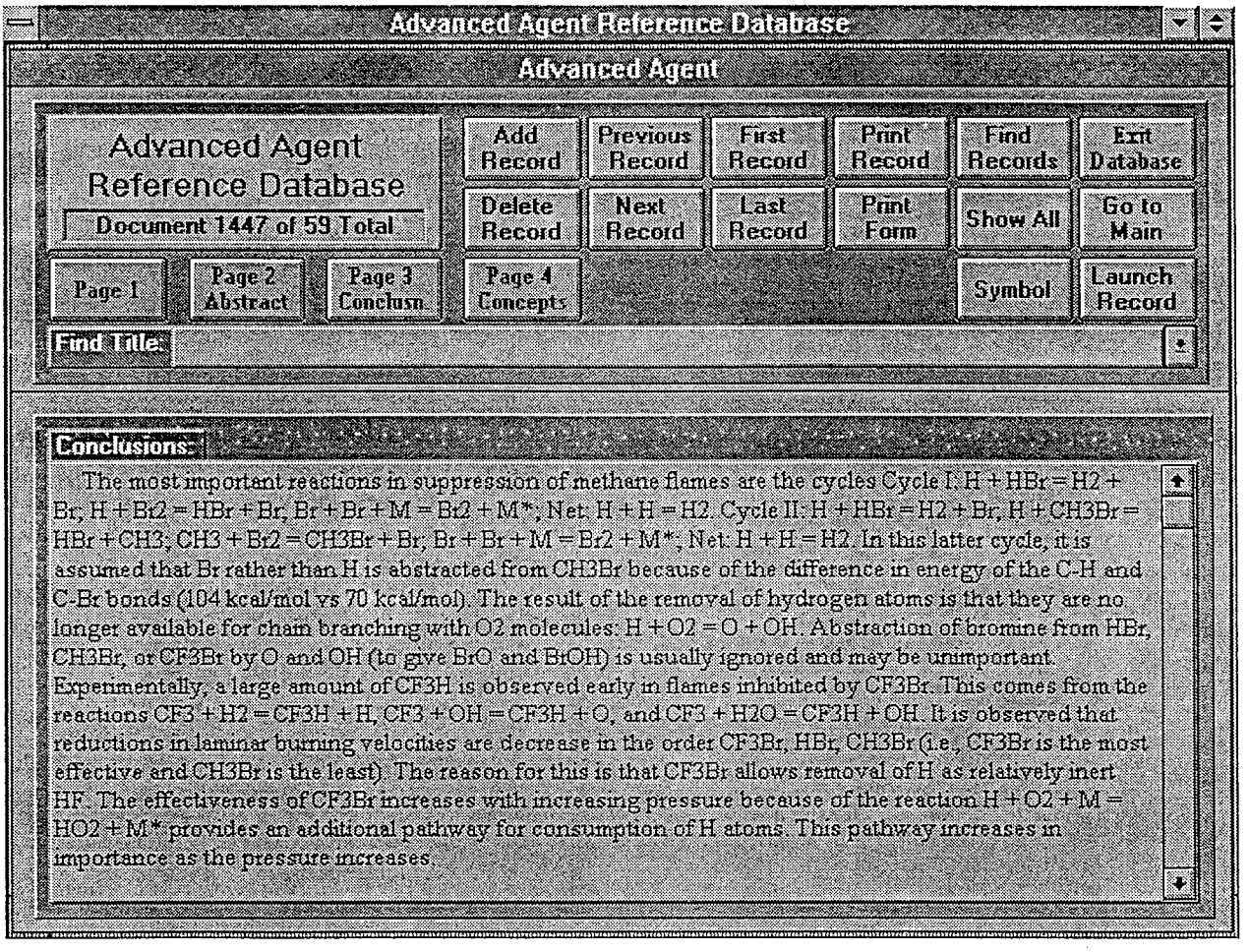

Figure 4. Form frmAdvanced Page 3.

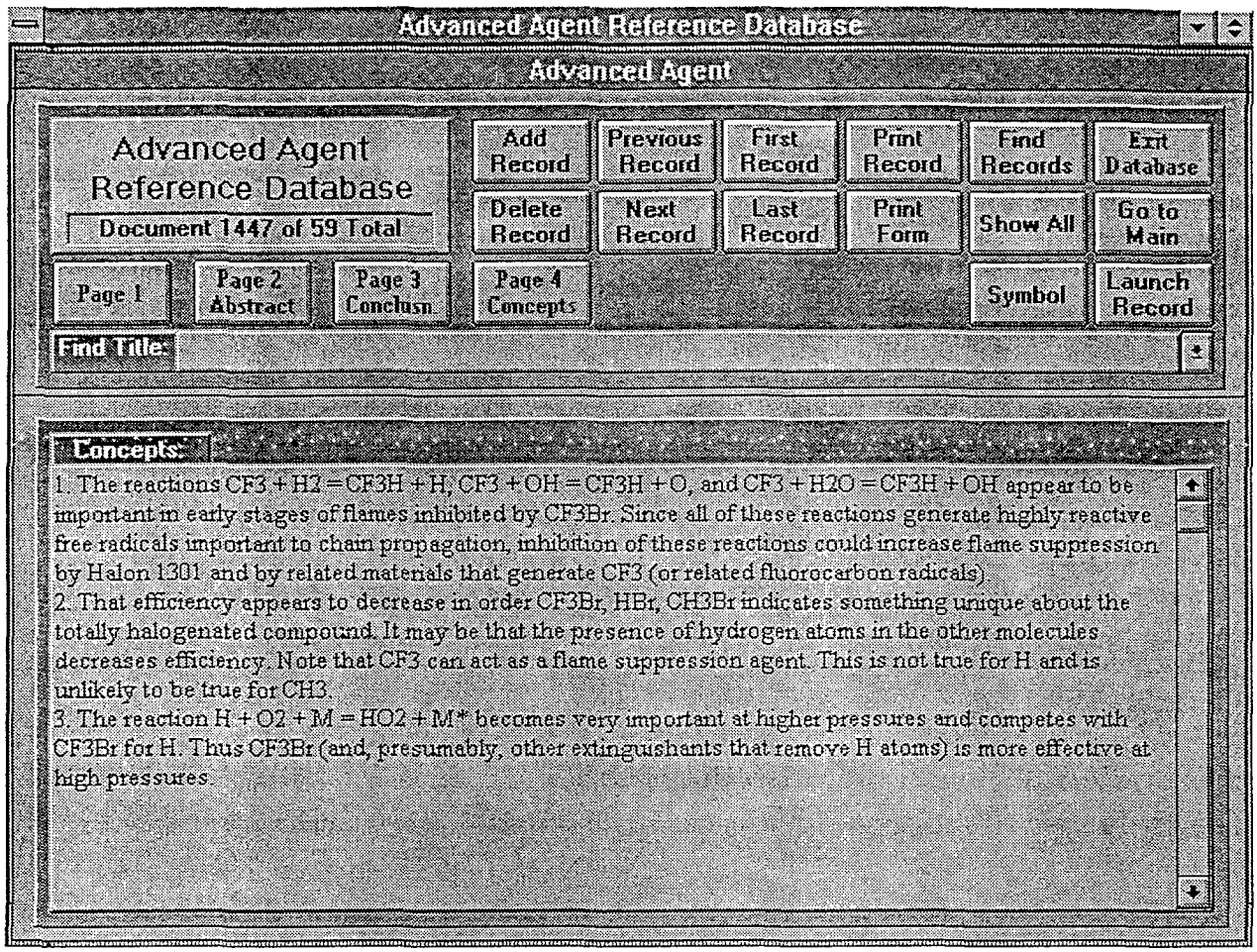

Figure 5. Form frmAdvanced Page 4.

The window under the Advanced Agent banner (Figure 5) indicates the reference number of the reference from the LIBRARY Database and the total number of references in the ADVANCED AGENT Database. After a find is used, the second number will display the number of records matching the find terms.

TABLE 10. BUTTONS IN FRMADVANCED.

Button	Function
	FUNCTION BUTTONS
"Add Record"	Opens an empty form to enter data for a new record
"Previous Record"	Opens the previous record
"First Record"	Moves to first record
"Print Record"	Prints the current record in the format of **rptAdvanced**
"Find Record"	Opens a popup which allows entry of search terms
"Exit Database"	Moves to screen from which the database was entered
"Delete Record"	Deletes the current record
"Next Record"	Moves to next record
"Last Record"	Moves to final non-empty record
"Print Form"	Prints the record as it is displayed on this form on 4 separate sheets (without the buttons displayed)
"Show All"	Removes all filters from the records
"Go To Main"	Returns to **frmSwitchboard**
"Symbol"	Opens up the Windows Character Map feature (may not operate with all systems)
"Launch Record"	Puts the current record in a format for launch in Word for Windows
	PAGE BUTTONS
"Page 1"	Displays first page of this form - general bibliographic data
"Page 2 Abstract"	Displays second page of this form - abstract of the reference
"Page 3 Conclusn"	Displays third page of this form - conclusions drawn from agents found in the reference
"Page 4 Concepts"	Displays fourth page of this form - concepts for new agents

The "find" bar opens a drop-down box that facilitates the selection of a record by author or title. Three "Subject" check boxes allow additional classification of the record. "Mechanisms," "Agents," "Fire Extinguishment," and "Properties" allows the classification of a record by its major subject, e.g, mechanisms of combustion, agent-specific information, concepts of fire extinguishment, or properties of candidate agents.

C. FIND FORM

The Find form(**frmFindMod**) is activated when the "Find" button on frmAdvanced is selected and allows the entering of terms for the database to conduct a search (Figure 6). After the term is entered, clicking on "OK" selects the record or records and displays the first record.

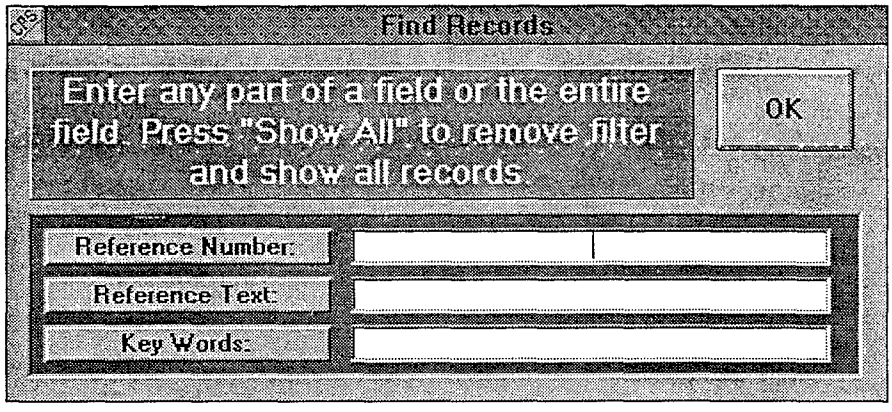

Figure 6. Form frmFindMod.

D. ADD RECORD FORM

The form to add records (**frmAddRecordMod**) is activated when the "Find" button on **frmAdvanced** is selected, which allows a single record from the LIBRARY Database to be selected for entry into the ADVANCED AGENT Database (Figure 7). The reference number is then entered into the box and "OK" selected. The "Add Record" button is deactivated in distributed copies since the LIBRARY Database must be used to add records.

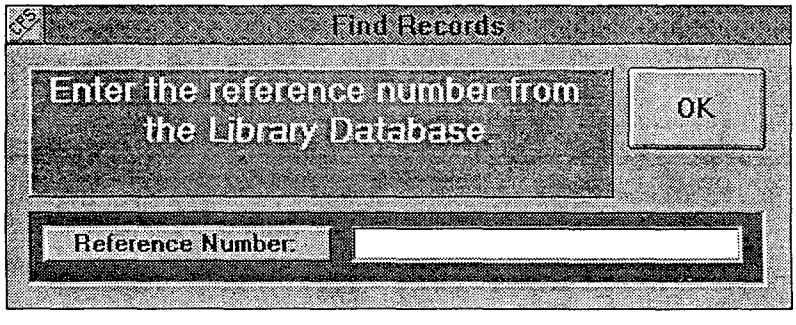

Figure 7. Form frmAddRecordMod.

SECTION IV
REPORTS

Two standardized reports are included with the database. The report **rptAdvanced** is produced on each record and contains the bibliographic record of each reference, the abstract, and the conclusions and concepts pages (Figure 8). Report **rptList** presents only the bibliographic listing of all reports (Figure 9).

Advanced Agent Database

Reference Number 6678

Casias, C. R., and McKinnon, J. T., "Mechanisms of Flame Quenching by Chlorine in Well-Stirred Reactors," Fourth International Congress on Toxic Byproducts of Combustion (University of California, Berkley Campus), Berkley, California, USA, 5-7 June, 1995.

Abstract:

This paper reports an evaluation of chlorine inhibition effects on the hydrocarbon combustion process using an elementary reaction mechanism consisting of 305 reactions and 77 species. The analysis was conducted by adding 1% (mole basis) elemental chlorine to fuel-lean and fuel-rich, C2H4/air mixtures, and running numerical simulations based on a perfectly-stirred reactor configuration. Analysis included the evaluation of: chlorine-catalyzed free radical recombination cycles carbon flux pathways, principal chain branching reactions, free radical flux pathways, chlorine flux pathways, and reaction exothermics. Additionally, this analysis incorporated the use of hypothetical molecule "deuterium" that possessed thermodynamic properties similar to hydrogen and chemical properties similar to chlorine. From this evaluation, it was determined that both chemical and thermal effects result from the addition of chlorine. The primary chemical effect results from suppression of the O-atom concentration. The primary thermal effect results from suppression of the highly exothermic H2O formation channel due to competition from HCL formation channels. Thermal effects were determined to be the mechanism primarily responsible for flame quenching in a well-stirred reactor.

Conclusions:

(1) For inhibition of halocarbon flames by chlorine-containing species, molecular modeling indicates that the usual halogen cycle giving recombination of hydrogen atoms to form diatomic hydrogen is not a significant process. Note that this may not be true for bromine or iodine.
(2) The following cycles (proposed by Fristom and Van Tiggelen) are, however, believed to be operative:

Concepts and Ideas:

Figure 8. Report rptAdvanced.

Advanced Agent References Database

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Figure 9. Report rptList.

SECTION V
LAUNCH PROCEDURES

Access and Word create a powerful combination for inclusion of the contents of the database in Microsoft Word reports and other documentation. In the version of the database resident on the CGET server, when the "Launch" button is pushed in the **frmAdvanced** or the "Launch all Document Information" button is pushed from **frmSwitchboard**, Word is opened and the selected data file is saved in the c:\winword\access subdirectory as access.atw. Word is then opened and a new document screen is displayed. The merged document can then be created using the "Tools Mailmerge Helper" selected through "Tools—Mailmerge" and following the directions to create the new document. Database fields may then be incorporated into the new document by clicking the "Insert Merge Field" button and selecting the desired fields. If the number of fields is too large to show fully on the screen, pushing <alt-shift-f> at the same time will display the same fields in a drop-down menu. Each field must then be entered separately.

The distributed version handles launches differently. When either of the launch buttons is pushed, Word is not opened and the user is given the choice of a destination directory and file name for the data file. The user can then open Word and incorporate the data into the Word document as described above.

SECTION VI
DISTRIBUTION

The ADVANCED AGENT Database has been designed for distribution to users who have Microsoft Windows installed on their computers but who may not have Microsoft Access. Any questions about this database should be addressed to:

Dr. Robert E. Tapscott
Center for Global Environmental Technologies
The University of New Mexico
901 University Blvd. SE
Albuquerque, New Mexico 87106-4339
Phone: (505) 272-7253
Fax: (505) 272-7203
e-mail: tapscott@nmeri_gate.unm.edu

The database is continuously updated, and periodic releases of the latest version are planned.

REFERENCES

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